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TERMINAL (ENTER 1, 2, 3, OR ?):2

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                 "Ask CAS" for self-help around the clock
NEWS
         SEP 09
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                 present
         DEC 08
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                 INPADOC: Legal Status data reloaded
NEWS
         SEP 29
                 DISSABS now available on STN
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NEWS
         OCT 10
                 PCTFULL: Two new display fields added
         OCT 21
NEWS
                 BIOSIS file reloaded and enhanced
        OCT 28
NEWS
                 BIOSIS file segment of TOXCENTER reloaded and enhanced
     8
NEWS 9
         NOV 24
                 MSDS-CCOHS file reloaded
NEWS 10
         DEC 08
                 CABA reloaded with left truncation
NEWS 11
         DEC 08
                 IMS file names changed
NEWS 12
        DEC 09
                 Experimental property data collected by CAS now available
                 in REGISTRY
         DEC 09
                 STN Entry Date available for display in REGISTRY and CA/CAplus
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         DEC 17
                 DGENE: Two new display fields added
NEWS 14
         DEC 18
                 BIOTECHNO no longer updated
NEWS 15
NEWS 16 DEC 19
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                 available
NEWS 17 DEC 22
                 Additional INPI reactions and pre-1907 documents added to CAS
                 databases
NEWS 18 DEC 22
                 IFIPAT/IFIUDB/IFICDB reloaded with new data and search fields
NEWS 19 DEC 22
                 ABI-INFORM now available on STN
NEWS EXPRESS DECEMBER 28 CURRENT WINDOWS VERSION IS V7.00, CURRENT
              MACINTOSH VERSION IS V6.0b(ENG) AND V6.0Jb(JP),
              AND CURRENT DISCOVER FILE IS DATED 23 SEPTEMBER 2003
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              General Internet Information
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Enter NEWS followed by the item number or name to see news on that specific topic.

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FILE 'BIOSIS' ENTERED AT 13:21:38 ON 07 JAN 2004 COPYRIGHT (C) 2004 BIOLOGICAL ABSTRACTS INC.(R)

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RECORDS LAST ADDED: 31 December 2003 (20031231/ED)

FILE RELOADED: 19 October 2003.

=> s ((calculat? or measure? or determin? or evaluat? or detect? or quantif? or analy?) (3w) amine)

238056 CALCULAT?

1065198 MEASURE?

1371383 DETERMIN?

860482 EVALUAT?

909534 DETECT?

108857 QUANTIF?

2062918 ANALY?

34117 AMINE

22007 AMINES 51442 AMINE

(AMINE OR AMINES)

L1 1402 ((CALCULAT? OR MEASURE? OR DETERMIN? OR EVALUAT? OR DETECT? OR QUANTIF? OR ANALY?) (3W) AMINE)

=>

=> s 11 same (ion)

MISSING OPERATOR L1 SAME

The search profile that was entered contains terms or nested terms that are not separated by a logical operator.

=> s 11 (p) ion

214764 ION

79206 IONS

267529 ION

(ION OR IONS)

L2

120 L1 (P) ION

=> s 12 and (prognosis or diagnosis)

99513 PROGNOSIS

1 PROGNOSISES

1563 PROGNOSES

100382 PROGNOSIS

(PROGNOSIS OR PROGNOSISES OR PROGNOSES)

589828 DIAGNOSIS

5 DIAGNOSISES

23783 DIAGNOSES

601490 DIAGNOSIS

(DIAGNOSIS OR DIAGNOSISES OR DIAGNOSES)

L3 1 L2 AND (PROGNOSIS OR DIAGNOSIS)

=> d 13 kwic

L3 ANSWER 1 OF 1 BIOSIS COPYRIGHT 2004 BIOLOGICAL ABSTRACTS INC. on STN

TI Novel application for ion mobility spectrometry: Diagnosing vaginal infections through measurement of biogenic

AB A method for **diagnosis** of bacterial vaginosis (BV) and other vaginal infections, based on **measurement** of biogenic **amines** present in a sample of vaginal fluid by **ion**

a two step procedure: addition of alkaline solution to release the. . biological matrices. A software package was developed for acquisition, storage and processing of the mobility spectra and for providing a diagnosis based on a table of rules. We report the results from testing of 210 samples of vaginal discharge fluid that. IT Parts, Structures, & Systems of Organisms IT vaginal fluid: reproductive system IT Diseases bacterial vaginosis: bacterial disease, reproductive system disease/female, diagnosis Vaginosis, Bacterial (MeSH) ΙT Diseases trichomoniasis: parasitic disease Trichomonas Infections (MeSH) Chemicals & Biochemicals TΤ biogenic amine => s 12 and (vagin?) 42495 VAGIN? 1 L2 AND (VAGIN?) L4=> d 14 ti L4ANSWER 1 OF 1 BIOSIS COPYRIGHT 2004 BIOLOGICAL ABSTRACTS INC. on STN Novel application for ion mobility spectrometry: Diagnosing TIvaginal infections through measurement of biogenic amines. => s (11 (p) (ion (w) mobility)) 214764 ION 79206 IONS 267529 ION (ION OR IONS) 52222 MOBILITY 4713 MOBILITIES 55499 MOBILITY (MOBILITY OR MOBILITIES) L_5 4 (L1 (P) (ION (W) MOBILITY)) => d 15 kwic 1-4 ANSWER 1 OF 4 BIOSIS COPYRIGHT 2004 BIOLOGICAL ABSTRACTS INC. on STN Novel application for ion mobility spectrometry: TIDiagnosing vaginal infections through measurement of biogenic amines. AΒ A method for diagnosis of bacterial vaginosis (BV) and other vaginal infections, based on measurement of biogenic amines present in a sample of vaginal fluid by ion mobility spectrometry (IMS) was developed. Sample introduction is through a two step procedure: addition of alkaline solution to release the volatile. ANSWER 2 OF 4 BIOSIS COPYRIGHT 2004 BIOLOGICAL ABSTRACTS INC. on STN L_5 ΤI Detection of biogenic amines in foods using ion mobility spectrometry and chemometrics. ANSWER 3 OF 4 BIOSIS COPYRIGHT 2004 BIOLOGICAL ABSTRACTS INC. on STN Determination of volatile biogenic amines in muscle TI food products by ion mobility spectrometry. The extent of spoilage of muscle food products was determined through AΒ measurement of volatile biogenic amines that emanated

mobility spectrometry (IMS) was developed. Sample introduction is through

,

from food samples. The release of the amines was enhanced by addition of a few drops of an alkaline solution and the amines were monitored by ion mobility spectrometry (IMS). The limit of detection of the method for trimethylamine (TMA) was 2 ng and the measurement was . . examined, and as expected, the higher the storage temperature the faster the spoilage. Thus, this pilot study shows that the measurement of biogenic amines can serve as an indicator for food spoilage or freshness.

ANSWER 4 OF 4 BIOSIS COPYRIGHT 2004 BIOLOGICAL ABSTRACTS INC. on STN L5 . . sensitive registration and identification of the organic nitrogen AB. base molecules in air and in mixtures of compounds for their chromatographic, ion mobility and mass-spectrometric analysis are presented. The main principles of the SI registration and identification of molecules are considered. The requirements. . . of the development of the effective and stable emitters, the simple-in-design diode SI detectors, the gas-chromatographic detectors, the SI gas analyzers of amines and the indicators and analyzers of narcotics including portable ones, SI ion mobility spectrometer and SI mass spectrometer are presented. They have a unique selectivity (up to 105-108 with respect to organic solvents).

=> d 15 1-4 iall

ANSWER 1 OF 4 BIOSIS COPYRIGHT 2004 BIOLOGICAL ABSTRACTS INC. on STN

ACCESSION NUMBER:

2003:66651 BIOSIS

DOCUMENT NUMBER:

PREV200300066651

TITLE:

; .

Novel application for ion mobility

spectrometry: Diagnosing vaginal infections through

measurement of biogenic amines.

AUTHOR (S):

Karpas, Zeev [Reprint Author]; Chaim, Walter; Gdalevsky, Rachel; Tilman, Boris; Lorber, Avi

Applicant

CORPORATE SOURCE:

Department of Analytical Chemistry, Nuclear Research

Center, P.O. Box 9001, Beer-Sheva, 84190, Israel

karpas4@netvision.net.il

SOURCE:

Analytica Chimica Acta, (9 December 2002) Vol. 474, No.

1-2, pp. 115-123. print.

ISSN: 0003-2670 (ISSN print).

DOCUMENT TYPE:

Article

LANGUAGE:

English

ENTRY DATE:

Entered STN: 29 Jan 2003

Last Updated on STN: 29 Jan 2003

ABSTRACT: A method for diagnosis of bacterial vaginosis (BV) and other vaginal infections, based on measurement of biogenic amines present in a sample of vaginal fluid by ion mobility spectrometry (IMS) was developed. Sample introduction is through a two step procedure: addition of alkaline solution to release the volatile amines followed by heating and acid addition for emanation of the semi-volatile amines. Addition of n-nonylamine vapors to the carrier gas stream helps control the ionization processes and enhances the selective response to amines, even in the complex environment of biological matrices. A software package was developed for acquisition, storage and processing of the mobility spectra and for providing a diagnosis based on a table of rules. We report the results from testing of 210 samples of vaginal discharge fluid that were diagnosed by a qynecologist according to the widely used reference method (Amsel test) and by the new IMS method. The new method is rapid (less than 2 min per sample), has a high sensitivity (few False Negatives) and specificity (few False Positives) with an accuracy of >95% for BV. The use of this method can reduce the incidence of misdiagnosis, particularly when trichomoniasis is confused with bacterial vaginosis.

CONCEPT CODE:

Pathology - Diagnostic 12504

Reproductive system - Physiology and biochemistry
Reproductive system - Pathology 16506 16504

Medical and clinical microbiology - Bacteriology

Parasitology - Medical 60504

Major Concepts INDEX TERMS:

Gynecology (Human Medicine, Medical Sciences);

Infection; Methods and Techniques

Parts, Structures, & Systems of Organisms INDEX TERMS:

vaginal fluid: reproductive system

INDEX TERMS: Diseases

bacterial vaginosis: bacterial disease, reproductive

system disease/female, diagnosis

Vaginosis, Bacterial (MeSH)

INDEX TERMS: Diseases

trichomoniasis: parasitic disease

Trichomonas Infections (MeSH)

Chemicals & Biochemicals INDEX TERMS:

biogenic amine

Methods & Equipment INDEX TERMS:

ion mobility spectrometry: clinical techniques,

diagnostic techniques, spectrum analysis techniques; Amsel test: clinical techniques, diagnostic techniques

Classifier ORGANISM:

> Hominidae 86215

Super Taxa

Primates; Mammalia; Vertebrata; Chordata; Animalia

Organism Name

human (common): host, female

Taxa Notes

Animals, Chordates, Humans, Mammals, Primates,

Vertebrates

ANSWER 2 OF 4 BIOSIS COPYRIGHT 2004 BIOLOGICAL ABSTRACTS INC. on STN

ACCESSION NUMBER: DOCUMENT NUMBER:

PREV200200521328

2002:521328 BIOSIS

TITLE:

. .

Detection of biogenic amines in foods using ion mobility spectrometry and

chemometrics.

AUTHOR (S):

Harrington, Peter de B. [Reprint author]; Schmitt, Nicholas

CORPORATE SOURCE:

C.; Atkinson, David A.; Ewing, Robert G. Department of Chemistry and Biochemistry, Center for

Intelligent Chemical Instrumentation, Clippinger Laboratories, Ohio University, Athens, OH, 45701, USA

Peter.Harrington@Ohio.edu

SOURCE:

Abstracts of Papers American Chemical Society, (2002) Vol.

224, No. 1-2, pp. AGFD 192. print.

Meeting Info.: 224th National Meeting of the American Chemical Society. Boston, MA, USA. August 18-22, 2002

CODEN: ACSRAL. ISSN: 0065-7727.

DOCUMENT TYPE:

Conference; (Meeting)

Conference; Abstract; (Meeting Abstract)

LANGUAGE:

English ENTRY DATE:

Entered STN: 9 Oct 2002

Last Updated on STN: 9 Oct 2002

CONCEPT CODE:

General biology - Symposia, transactions and proceedings

00520

Food technology - General and methods

INDEX TERMS:

Major Concepts

Foods; Methods and Techniques

INDEX TERMS:

Chemicals & Biochemicals

biogenic amines; cadaverine; putrescine

INDEX TERMS:

Methods & Equipment

ion mobility spectrometry: analytical method

INDEX TERMS: Miscellaneous Descriptors

chemometrics; food products: flavor, quality, spoilage;

food safety; Meeting Abstract

REGISTRY NUMBER:

462-94-2 (cadaverine) 110-60-1 (putrescine)

ANSWER 3 OF 4 BIOSIS COPYRIGHT 2004 BIOLOGICAL ABSTRACTS INC. on STN

ACCESSION NUMBER: 2002:520747 BIOSIS PREV200200520747 DOCUMENT NUMBER:

Determination of volatile biogenic amines TITLE:

in muscle food products by ion mobility

spectrometry.

Karpas, Zeev [Reprint author]; Tilman, Boris; Gdalevsky, AUTHOR (S):

Rachel; Lorber, Avraham

Analytical Chemistry Department, Nuclear Research Center, CORPORATE SOURCE:

Negev, P.O. Box 9001, Beer-Sheva, 84190, Israel

Applicant

karpas4@netvision.net.il

Analytica Chimica Acta, (22 July, 2002) Vol. 463, No. 2, SOURCE:

pp. 155-163. print.

CODEN: ACACAM. ISSN: 0003-2670.

DOCUMENT TYPE: Article English LANGUAGE:

freshness.

. .

ENTRY DATE:

Entered STN: 9 Oct 2002 Last Updated on STN: 9 Oct 2002

ABSTRACT: The extent of spoilage of muscle food products was determined through

of volatile biogenic amines that emanated from ***measurement***

food samples. The release of the amines was enhanced by addition of a few

drops of an alkaline solution and the amines were monitored by ion

mobility spectrometry (IMS). The limit of detection of the method for trimethylamine (TMA) was 2 ng and the measurement was completed within <2 min with short and long term reproducibility of 15 and 25%, respectively, for

replicate samples. The method provides qualitative information as it distinguishes between different amines, as well as quantitative data for the key compounds. A good correlation was found between the IMS results and the microorganism populations in microbiological cultures. The effects of storage

time and temperature and of the type of meat on the formation of biogenic amines were examined, and as expected, the higher the storage temperature the faster the spoilage. Thus, this pilot study shows that the measurement of biogenic amines can serve as an indicator for food spoilage or

Food technology - General and methods CONCEPT CODE:

Food technology - Meats and meat by-products 13516

Muscle - Physiology and biochemistry

INDEX TERMS: Major Concepts

Foods; Methods and Téchniques

Parts, Structures, & Systems of Organisms INDEX TERMS:

muscle: muscular system

Chemicals & Biochemicals INDEX TERMS:

trimethylamine; volatile biogenic amines: determination

Methods & Equipment INDEX TERMS:

ion mobility spectrometry: Spectrum Analysis Techniques,

determination method

INDEX TERMS: Miscellaneous Descriptors

food spoilage; muscle food product: meat product

REGISTRY NUMBER: 75-50-3 (trimethylamine)

BIOSIS COPYRIGHT 2004 BIOLOGICAL ABSTRACTS INC. on STN ANSWER 4 OF 4

2000:540557 BIOSIS ACCESSION NUMBER:

DOCUMENT NUMBER: PREV200000540557

TITLE: Surface-ionization methods and devices of indication and

identification of nitrogen-containing base molecules.

Rasulev, U. Kh. [Reprint author]; Khasanov, U.; Palitcin, AUTHOR (S):

Arifov Institute of Electronics, Uzbek Academy of Sciences CORPORATE SOURCE:

Academgorodok, F. Khojaeva 33, 700143, Tashkent:

root@ariel.tashkent.su, Uzbekistan

Journal of Chromatography A, (27 October, 2000) Vol. 896, SOURCE:

No. 1-2, pp. 3-18. print. CODEN: JOCRAM. ISSN: 0021-9673.

DOCUMENT TYPE: Article LANGUAGE:

1 .

English

ENTRY DATE:

Entered STN: 13 Dec 2000

Last Updated on STN: 11 Jan 2002

ABSTRACT: The results of the development of methods and devices based on the effect of surface ionization (SI) and intended for the selective and sensitive registration and identification of the organic nitrogen base molecules in air and in mixtures of compounds for their chromatographic, ion ***mobility*** and mass-spectrometric analysis are presented. principles of the SI registration and identification of molecules are considered. The requirements that must be satisfied by devices implementing these principles are stated. The examples of the development of the effective and stable emitters, the simple-in-design diode SI detectors, the gas-chromatographic detectors, the SI gas analyzers of amines and the indicators and analyzers of narcotics including portable ones, SI mobility spectrometer and SI mass spectrometer are ***ion*** They have a unique selectivity (up to 105-108 with respect to presented. organic solvents) and ionization efficiency (up to apprx2cntdot10-1) of amines and their derivatives, including the degradation products of chemical warfare agents, tobacco alkoloids, triazine herbicides, narcotics and other abused medicinal preparations, as well as the sensitivity of up to 6 C/g and picogram level detection limits with a response dynamic range of 5-8 orders of magnitude.

CONCEPT CODE:

Biochemistry studies - General 10060

INDEX TERMS:

Major Concepts

Biochemistry and Molecular Biophysics; Equipment, Apparatus, Devices and Instrumentation; Methods and

Techniques

INDEX TERMS:

Chemicals & Biochemicals

abused medicinal preparations; amines: derivatives; base molecules: identification, nitrogen-containing, registration; chemical warfare agents: degradation products; mixtures of compounds; narcotics: degradation products; tobacco alkaloids: degradation products;

triazine herbicides: degradation products

INDEX TERMS:

Methods & Equipment

DB-5 capillary columns: J&W, laboratory equipment; HP-5890 chromatograph: Hewlett-Packard, laboratory equipment; chromato-mass spectrometer HP-6890: Hewlett-Packard, laboratory equipment; chromatography: Chromatographic Techniques, analytical method; gas-chromatographic detectors: laboratory equipment; ion mobility spectrometry: Spectrum Analysis Techniques, analytical method; magnetic mass spectrometer MI-1201V: NPO Elektron, laboratory equipment; mass-spectrometry: Spectrum Analysis Techniques, analytical method; model 3 LKhM-8MD chromatograph: OKBA, laboratory equipment; model 550 Tsvet-500M chromatograph: OKBA, laboratory equipment; series 104 Pay-Unicam chromatograph: Hewlett-Packard, laboratory equipment; simple-in-design diode surface ionization detectors: laboratory equipment; surface ionization gas analyzers: laboratory equipment; surface ionization ion mobility spectrometer: laboratory equipment; surface ionization mass spectrometer: laboratory equipment; surface-ionization: Spectrum Analysis Techniques, analytical method; surface-ionization devices: laboratory equipment

INDEX TERMS:

Miscellaneous Descriptors air; ionization efficiency

=> s (11 and (ion (w) mobility)
UNMATCHED LEFT PARENTHESIS '(L1'
The number of right parentheses in a query must be equal to the number of left parentheses.

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=> s (l1 and (ion (w) mobility))
        214764 ION
         79206 IONS
        267529 ION
                 (ION OR IONS)
         52222 MOBILITY
          4713 MOBILITIES
         55499 MOBILITY
                 (MOBILITY OR MOBILITIES)
           266 ION (W) MOBILITY
             4 (L1 AND (ION (W) MOBILITY))
L6
=> d l6 ti 1-4
     ANSWER 1 OF 4 BIOSIS COPYRIGHT 2004 BIOLOGICAL ABSTRACTS INC. on STN
     Novel application for ion mobility spectrometry:
ΤI
     Diagnosing vaginal infections through measurement of biogenic
     amines.
     ANSWER 2 OF 4 BIOSIS COPYRIGHT 2004 BIOLOGICAL ABSTRACTS INC. on STN
1.6
ΤТ
     Detection of biogenic amines in foods using
     ion mobility spectrometry and chemometrics.
     ANSWER 3 OF 4 BIOSIS COPYRIGHT 2004 BIOLOGICAL ABSTRACTS INC. on STN
Ь6
     Determination of volatile biogenic amines in muscle
TТ
     food products by ion mobility spectrometry.
     ANSWER 4 OF 4 BIOSIS COPYRIGHT 2004 BIOLOGICAL ABSTRACTS INC. on STN
_{\rm L6}
TТ
     Surface-ionization methods and devices of indication and identification of
     nitrogen-containing base molecules.
=> s (l1 and spectrometry)
         86516 SPECTROMETRY
            92 SPECTROMETRIES
         86575 SPECTROMETRY
                 (SPECTROMETRY OR SPECTROMETRIES)
L7
           122 (L1 AND SPECTROMETRY)
=> s 17 and (prognosis or diagnosis or disease or patholog? or condition)
         99513 PROGNOSIS
             1 PROGNOSISES
          1563 PROGNOSES
        100382 PROGNOSIS
                 (PROGNOSIS OR PROGNOSISES OR PROGNOSES)
        589828 DIAGNOSIS
             5 DIAGNOSISES
         23783 DIAGNOSES
        601490 DIAGNOSIS
                 (DIAGNOSIS OR DIAGNOSISES OR DIAGNOSES)
       2227397 DISEASE
       1536285 DISEASES
       2389522 DISEASE
                 (DISEASE OR DISEASES)
       1468485 PATHOLOG?
        137613 CONDITION
        609164 CONDITIONS
        718370 CONDITION
                 (CONDITION OR CONDITIONS)
L8
            24 L7 AND (PROGNOSIS OR DIAGNOSIS OR DISEASE OR PATHOLOG? OR CONDIT
               ION)
=> s 18 and ion
        214764 ION
```

79206 IONS

. .

=> d 19 1-7 kwic

٠. .

L9 ANSWER 1 OF 7 BIOSIS COPYRIGHT 2004 BIOLOGICAL ABSTRACTS INC. on STN
AB. . . a mixed cation exchange reversed-phase resin. The identity of 4-ABP was confirmed by both HPLC with electrospray ionization tandem mass spectrometry (HPLC-ESI-MS/MS) and gas chromatography with negative ion chemical ionization mass spectrometry (GC-NICI-MS) following chemical derivatization with pentafluoropropionic anhydride (PFPA). The levels of 4-ABP ranged from not detectable (<0.29 parts per billion. . . is present in some hair dyes. Studies on dermal absorption and bioavailability of 4-ABP from hair dyes are required to determine if this aromatic amine contributes to the increased risk of bladder cancer reported in frequent users of hair dyes.

IT Major Concepts

Cosmetics; Toxicology; Tumor Biology

IT Diseases

bladder cancer: neoplastic disease, urologic disease Bladder Neoplasms (MeSH)

IT Chemicals & Biochemicals

1,4-phenylenediamine; 4-aminobiphenyl: carcinogen; DNA adducts; aminobiphenyl derivatives: identification; commercial hair dyes; hexane; pentafluoropropionic anhydride

- L9 ANSWER 2 OF 7 BIOSIS COPYRIGHT 2004 BIOLOGICAL ABSTRACTS INC. on STN Novel application for ion mobility spectrometry:

 Diagnosing vaginal infections through measurement of biogenic amines.
- AB A method for diagnosis of bacterial vaginosis (BV) and other vaginal infections, based on measurement of biogenic amines present in a sample of vaginal fluid by ion mobility spectrometry (IMS) was developed. Sample introduction is through a two step procedure: addition of alkaline solution to release the volatile amines. . . biological matrices. A software package was developed for acquisition, storage and processing of the mobility spectra and for providing a diagnosis based on a table of rules. We report the results from testing of 210 samples of vaginal discharge fluid that. . .

Infection; Methods and Techniques

IT Parts, Structures, & Systems of Organisms vaginal fluid: reproductive system

IT Diseases

ΙT

bacterial vaginosis: bacterial disease, reproductive system
disease/female, diagnosis
Vaginosis, Bacterial (MeSH)

IT Diseases

trichomoniasis: parasitic disease Trichomonas Infections (MeSH)

IT Chemicals & Biochemicals

biogenic amine

IT Methods & Equipment

ion mobility spectrometry: clinical techniques, diagnostic techniques, spectrum analysis techniques; Amsel test: clinical techniques, diagnostic techniques

- L9 ANSWER 3 OF 7 BIOSIS COPYRIGHT 2004 BIOLOGICAL ABSTRACTS INC. on STN
- TI Atmospheric pressure ionization time-of-flight mass **spectrometry** coupled with fast liquid chromatography for quantitation and accurate mass measurement of five pharmaceutical drugs in human plasma.
- AB The quantitative determination and accurate mass measurement of five tricyclic amine pharmaceutical drugs (doxepin, desipramine,

imipramine, amitriptyline and trimipramine) fortified in human plasma within a per sample run time of 18 s was accomplished by atmospheric pressure ionization (API) time-of-flight (TOF) mass spectrometry using a turboIonspray liquid chromatography/mass spectrometry (LC/MS) interface coupled with high-performance liquid chromatography (HPLC). The relatively short HPLC separation (18 s) was achieved using a . maintained at a flow-rate of 1.4 ml min-1. An acquisition speed of 0.2 s per spectrum accommodates these fast separation conditions. This method employs a one-step liquid-liquid extraction procedure to isolate the five tricyclic amines from biological matrix components The overall. . . and accuracy (0.2-14.5%) were obtained. The linear dynamic range was extended to 200 based on a software upgrade for correcting ion current detection saturation. The accurate masses of the five tricyclic amines were determined by on-line LC/TOFMS analyses of biological extracts. Equipment

API-TOF mass spectrometer: equipment; high performance liquid chromatography [HPLC]: liquid chromatography, separation method; liquid chromatography-atmospheric pressure ionization time-of-flight mass spectrometry [LC-API-TOF-MS]: Spectrum Analysis Techniques, analytical method; liquid-liquid extraction: Extraction, Isolation, Purification and Separation Techniques, extraction method

- L9 ANSWER 4 OF 7 BIOSIS COPYRIGHT 2004 BIOLOGICAL ABSTRACTS INC. on STN Determination of heterocyclic aromatic amines in meat extracts by liquid chromatography-ion-trap atmospheric pressure chemical ionization mass spectrometry.
- AB When protein-rich foods are processed under normal cooking conditions, heterocyclic aromatic amines (HAAs) can be generated at a few parts per billion level. In this work, we have analyzed. . . time has been greatly reduced. Problems derived from the less exhaustive purification of the extract have been solved by using MS(ion trap) detection. The RSD for quantification ranged from 2.1% to 5.1% for run-to-run precision and from 5.2% to 11% for. . .

 IT Methods & Equipment

HPLC [high performance liquid chromatography]: liquid chromatography, separation method; Pharmacia LKB HPLC system: equipment; ion trap atmospheric pressure chemical ionization mass spectrometry [IT-APCI-MS]: analytical method, spectroscopic techniques: CB

IT Miscellaneous Descriptors

meat: meat

IT

- L9 ANSWER 5 OF 7 BIOSIS COPYRIGHT 2004 BIOLOGICAL ABSTRACTS INC. on STN Liquid chromatography-atmospheric-pressure chemical ionization mass spectrometry as a routine method for the analysis of mutagenic amines in beef extracts.
- AB A liquid chromatography-mass spectrometry (LC-MS) method using atmospheric-pressure chemical ionization as interface was developed for the simultaneous determination of 14 heterocyclic aromatic amines and. . . spectra were optimized, and the effect of the variation of cone voltage on the mass spectra was studied. The (M+H)+ ions and some fragments produced in the source were observed in the mass spectra when several extraction voltages were applied. Quality parameters (run-to-run and day-to-day reproducibility, intervals of linearity, and limits of detection) were studied in the optimum working conditions. The method was used to analyze the heterocyclic amines present in a commercial beef extracts. Therefore, a solid-phase extraction clean-up procedure was performed prior to the LC-MS analysis due. . .
- IT Miscellaneous Descriptors
 ANALYSIS; ANALYTICAL METHOD; BEEF EXTRACTS; FOOD MUTAGEN; FOODS;
 HARMAN; HETEROCYCLIC AMINES; LIQUID CHROMATOGRAPHY-ATMOSPHERIC PRESSURE
 CHEMICAL IONIZATION MASS SPECTROMETRY; METHODOLOGY;
 NORHARMAN; TOXICOLOGY; 2-AMINO-1-METHYL-6-PHENYLIMIDAZO(4,5-B)PYRIDINE;
 2-AMINO-3-METHYL-9H-PYRIDO(2,3-B)INDOLE; 2-AMINO-3-METHYLIMIDAZO(4,5-

F) QUINOLINE; 2-AMINO-3,4-DIMETHYLIMIDAZO(4,5-F) QUINOLINE; 2-AMINO-3,4,7,8-TETRAMETHYLIMIDAZO(4,5-F) QUINOXALINE; 2-AMINO-3,4,8-TRIMETHYLIMIDAZO(4,5-F) QUINOXALINE; 2-AMINO-3,7,8-TRIMETHYLIMIDAZO(4,5-F) QUINOXALINE; 2-AMINO-3,8-DIMETHYLIMIDAZO(4,5-F) QUINOXALINE; 2-AMINO-6-METHYLDIPYRIDO(1,2-A:3',2'-D) IMIDAZOLE; 2-AMINO-9H-PYRIDO(2,3-B) INDOLE; 3-AMINO-1-METHYL-5H-PYRIDO(4,3-B) INDOLE; 3-AMINO-1,4-DIMETHYL-5H-PYRIDO(4,3-B) INDOLE

- L9 ANSWER 6 OF 7 BIOSIS COPYRIGHT 2004 BIOLOGICAL ABSTRACTS INC. on STN
- TI Determination of heterocyclic amines by pneumatically assisted electrospray liquid chromatography-mass spectrometry.
- AB Electrospray ionization mass spectrometry was applied to the study of the amines IQ, Trp-P-1, Trp-P-2, PhIP and A-alpha-C and the co-mutagens harman and norharman.... The results obtained on a triple quadrupole mass spectrometer equipped with a pneumatically assisted electrospray source are reported. The chromatographic conditions were optimized with a reversed-phase column (1 mm I.D.) using acetonitrile-5 mM ammonium acetate (pH 6.7) (50:50) as the mobile. . . of 50 mu-l min-1. Different parameters influencing the mass spectra were investigated. For these compounds (M + H) + in the positive-ion mode and also some fragments produced through collisionally activated decomposition in the interface were observed. Detection limits of 5.4-44 pg were obtained for standard solutions of these amines. Analysis of a meat extract was performed by HPLC-MS using single-ion monitoring after a solid-phase extraction clean-up.
- L9 ANSWER 7 OF 7 BIOSIS COPYRIGHT 2004 BIOLOGICAL ABSTRACTS INC. ON STN
 TI DETERMINATION OF PRIMARY AND SECONDARY ALIPHATIC AMINES IN THE ENVIRONMENT
 AS SULFONAMIDE DERIVATIVES BY GAS CHROMATOGRAPHY-MASS SPECTROMETRY
- AB. . . developed. A standard solution of amines was added to river water, sea water and sea sediment, and distilled under alkaline conditions. The distillate was reacted with benzenesulphonyl chloride to form the corresponding sulphonamides. After extracting the derivatives into dichloromethane, the organic layer was concentrated to a definite volume. The determination was carried out by GC-MS with selected-ion monitoring. The detection limits of amines in water and sediment were 0.02-2 .mu.g/l and 0.5-50 .mu.g/kg, respectively. The recoveries were 68.4-98.8%.

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L9 ANSWER 1 OF 7 BIOSIS COPYRIGHT 2004 BIOLOGICAL ABSTRACTS INC. on STN

ACCESSION NUMBER: 2003:458361 BIOSIS DOCUMENT NUMBER: PREV200300458361

TITLE: Identification of aminobiphenyl derivatives in commercial

hair dyes.

AUTHOR(S): Turesky, Robert J. [Reprint Author]; Freeman, James P.;

Holland, Ricky D.; Nestorick, Daniel M.; Miller, Dwight W.;

Ratnasinghe, D. Luke; Kadlubar, Fred F.

CORPORATE SOURCE: Division of Chemistry, National Center for Toxicological

Research, 3900 NCTR Road, Jefferson, AR, 72079, USA

RTuresky@nctr.fda.gov

SOURCE: Chemical Research in Toxicology, (September 2003) Vol. 16,

No. 9, pp. 1162-1173. print.

ISSN: 0893-228X (ISSN print).

DOCUMENT TYPE: Article LANGUAGE: English

ENTRY DATE: Entered STN: 8 Oct 2003

Last Updated on STN: 8 Oct 2003

ABSTRACT:A recent epidemiological study suggested that aromatic amines present in hair dyes may contribute to an increased risk of bladder cancer (Gago-Dominguez, et al. (2003) Carcinogenesis 24, 483-489). Moreover, a preliminary study linked frequent hair dye usage with elevated levels of DNA

adducts of 4-aminobiphenyl (4-ABP) in human epithelial breast cells (Gorlewska, et al. Proc. Am. Assoc. Cancer Res. 43, 1018-1019). Therefore, we sought to determine if 4-ABP, a recognized human urinary bladder carcinogen, is present in commercial hair dyes. 4-ABP was isolated from dyes by solvent extraction with hexane, followed by silica gel chromatography, either with or without chemical treatment of the extract with Zinc/HCl, and a final purification with a mixed cation exchange reversed-phase resin. The identity of 4-ABP was confirmed by both HPLC with electrospray ionization tandem mass ***spectrometry*** (HPLC-ESI-MS/MS) and gas chromatography with negative ***ion*** chemical ionization mass spectrometry (GC-NICI-MS) following chemical derivatization with pentafluoropropionic anhydride (PFPA). The levels of 4-ABP ranged from not detectable (<0.29 parts per billion (ppb)) up to 12.8 ppb. The noncarcinogenic isomer 2-aminobiphenyl (2-ABP) was also found at quantities up to 310 ppb. 4-ABP was detected in eight of the 11 hair dyes and found in black, red, and blonde hair dyes but not in brown hair dyes. 1,4-Phenylenediamine (PPD) is a key constituent for color development of many permanent hair dyes. Some batches of chemical research grade PPD were contaminated with 4-ABP (up to 500 ppb) and 2-ABP (up to 70 parts per million) and may be a source of ABP contamination in hair dyes. These analytical data demonstrate that 4-ABP is present in some hair dyes. Studies on dermal absorption and bioavailability of 4-ABP from hair dyes are required to ***determine*** if this aromatic amine contributes to the increased risk of bladder cancer reported in frequent users of hair dyes. CONCEPT CODE: General biology - Miscellaneous

Biochemistry studies - Nucleic acids, purines and

pyrimidines 10062

Urinary system - Pathology 15506 Toxicology - General and methods 22501

Neoplasms - Pathology, clinical aspects and systemic

effects 24004

Neoplasms - Carcinogens and carcinogenesis 24007

INDEX TERMS:

Major Concepts

Cosmetics; Toxicology; Tumor Biology Diseases

INDEX TERMS:

bladder cancer: neoplastic disease, urologic

disease

Bladder Neoplasms (MeSH)

INDEX TERMS:

Chemicals & Biochemicals

1,4-phenylenediamine; 4-aminobiphenyl: carcinogen; DNA adducts; aminobiphenyl derivatives: identification; commercial hair dyes; hexane; pentafluoropropionic

anhydride

ORGANISM:

Classifier

Hominidae 86215

Super Taxa

Primates; Mammalia; Vertebrata; Chordata; Animalia

Organism Name human (common)

Taxa Notes

Animals, Chordates, Humans, Mammals, Primates,

Vertebrates

REGISTRY NUMBER:

106-50-3 (1,4-phenylenediamine)

92-67-1 (4-aminobiphenyl)

41674-04-8D (aminobiphenyl derivatives)

110-54-3 (hexane)

356-42-3 (pentafluoropropionic anhydride)

L9 ANSWER 4 OF 7

BIOSIS COPYRIGHT 2004 BIOLOGICAL ABSTRACTS INC. on STN

ACCESSION NUMBER: DOCUMENT NUMBER:

2000:151485 BIOSIS PREV200000151485

TITLE:

Determination of heterocyclic aromatic

amines in meat extracts by liquid chromatographyion-trap atmospheric pressure chemical ionization

mass spectrometry.

AUTHOR(S): Toribio, F.; Moyano, E.; Puignou, L. [Reprint author];

Galceran, M. T.

CORPORATE SOURCE:

Departament de Quimica Analitica, Universitat de Barcelona,

Diagonal 647, 08028, Barcelona, Spain

SOURCE:

Journal of Chromatography A, (Feb. 11, 2000) Vol. 866, No.

1-2, pp. 307-317. print.

CODEN: JOCRAM. ISSN: 0021-9673.

DOCUMENT TYPE: LANGUAGE:

Article English

ENTRY DATE:

Entered STN: 19 Apr 2000

Last Updated on STN: 4 Jan 2002

ABSTRACT: When protein-rich foods are processed under normal cooking ***conditions*** , heterocyclic aromatic amines (HAAs) can be generated at a few parts per billion level. In this work, we have analyzed the HAAs present in a lyophilized meat extract by means of a simplified solid-phase extraction procedure. All the analytes were collected in a single extract with recoveries in the range of 45.6-75.2%, so the analysis time has been greatly reduced. Problems derived from the less exhaustive purification of the extract have been solved by using MS(ion trap) detection. The RSD for quantification ranged from 2.1% to 5.1% for run-to-run precision and from 5.2% to 11% for day-to-day precision. The limits of detection for standard solutions ranged from 20 to 150 pg injected. For the meat extract analyzed limits of detection from 0.9 to 11.2 ng g-1 were obtained. Results of the quantification are in agreement with those obtained using different clean-up procedures.

CONCEPT CODE:

Toxicology - Foods, food residues, additives and

preservatives 22502

Biochemistry methods - General 10050 Biochemistry studies - General 10060

Biophysics - General 10502

Food technology - General and methods 13502

INDEX TERMS:

Major Concepts

Biochemistry and Molecular Biophysics; Foods; Methods

and Techniques; Toxicology

INDEX TERMS:

Chemicals & Biochemicals

heterocyclic aromatic amines: Toronto Research Chemicals Inc., analysis, food residue, meat extracts, separation Methods & Equipment

INDEX TERMS:

HPLC [high performance liquid chromatography]: liquid chromatography, separation method; Pharmacia LKB HPLC

system: equipment; ion trap atmospheric

pressure chemical ionization mass spectrometry [IT-APCI-MS]: analytical method, spectroscopic

techniques: CB

INDEX TERMS:

Miscellaneous Descriptors

meat: meat

ANSWER 5 OF 7 BIOSIS COPYRIGHT 2004 BIOLOGICAL ABSTRACTS INC. on STN

ACCESSION NUMBER: DOCUMENT NUMBER:

1997:463516 BIOSIS PREV199799762719

TITLE:

Liquid chromatography-atmospheric-pressure chemical ionization mass spectrometry as a routine method

for the analysis of mutagenic amines in

beef extracts.

AUTHOR(S):

Pais, P.; Moyano, E.; Puignou, L.; Galceran, M. T. [Reprint

author]

CORPORATE SOURCE:

Dep. Quimica Analitica, Univ. Barcelona, Av. Diagonal 647,

08028 Barcelona, Spain

SOURCE:

Journal of Chromatography A, (1997) Vol. 778, No. 1-2, pp.

207-218.

CODEN: JOCRAM. ISSN: 0021-9673.

DOCUMENT TYPE:

Article English

LANGUAGE: ENTRY DATE:

Entered STN: 27 Oct 1997

Last Updated on STN: 27 Oct 1997

ABSTRACT: A liquid chromatography-mass spectrometry (LC-MS) method using atmospheric-pressure chemical ionization as interface was developed for the simultaneous determination of 14 heterocyclic aromatic amines and related compounds in beef extracts. The separation was performed on a conventional C-18 column using a binary mobile phase composed of acetonitrile and 50 mM ammonium acetate at pH 5.7, and elution was carried out in gradient mode. Several parameters influencing the mass spectra were optimized, and the effect of the variation of cone voltage on the mass spectra was studied. The (M+H)+ and some fragments produced in the source were observed in the mass spectra when several extraction voltages were applied. Quality parameters (run-to-run and day-to-day reproducibility, intervals of linearity, and limits of detection) were studied in the optimum working conditions. The method was used to analyze the heterocyclic amines present in a commercial beef extracts. Therefore, a solid-phase extraction clean-up procedure was performed prior to the LC-MS analysis due to the complexity of the sample and the compounds Glu-P-1, Harman, Norharman and A-alpha-C were identified in the samples at ppb levels and successfully confirmed using in-source fragmentation. Biochemistry methods - General CONCEPT CODE: Biophysics - Methods and techniques Food technology - Meats and meat by-products 13516 Food technology - Evaluations of physical and chemical properties 13530 Toxicology - Foods, food residues, additives and preservatives 22502 Major Concepts INDEX TERMS: Biochemistry and Molecular Biophysics; Foods; Methods and Techniques; Toxicology Chemicals & Biochemicals INDEX TERMS: 2-AMINO-3-METHYLIMIDAZO(4,5-F)QUINOLINE; 2-AMINO-3,4-DIMETHYLIMIDAZO(4,5-F)QUINOLINE; 2-AMINO-3,8-DIMETHYLIMIDAZO(4,5-F)QUINOXALINE; 3-AMINO-1,4-DIMETHYL-5H-PYRIDO(4,3-B)INDOLE; 3-AMINO-1-METHYL-5H-PYRIDO (4,3-B) INDOLE; 2-AMINO-6-METHYLDIPYRIDO(1,2-A:3',2'-D)IMIDAZOLE; HARMAN; NORHARMAN Miscellaneous Descriptors INDEX TERMS: ANALYSIS; ANALYTICAL METHOD; BEEF EXTRACTS; FOOD MUTAGEN; FOODS; HARMAN; HETEROCYCLIC AMINES; LIQUID CHROMATOGRAPHY-ATMOSPHERIC PRESSURE CHEMICAL IONIZATION MASS SPECTROMETRY; METHODOLOGY; NORHARMAN; TOXICOLOGY; 2-AMINO-1-METHYL-6-PHENYLIMIDAZO(4,5-B) PYRIDINE; 2-AMINO-3-METHYL-9H-PYRIDO(2,3-B) INDOLE; 2-AMINO-3-METHYLIMIDAZO(4,5-F)QUINOLINE; 2-AMINO-3, 4-DIMETHYLIMIDAZO(4,5-F)QUINOLINE; 2-AMINO-3,4,7,8-TETRAMETHYLIMIDAZO(4,5-F)QUINOXALINE; 2-AMINO-3,4,8-TRIMETHYLIMIDAZO(4,5-F)QUINOXALINE; 2-AMINO-3,7,8-TRIMETHYLIMIDAZO(4,5-F)QUINOXALINE; 2-AMINO-3,8-DIMETHYLIMIDAZO(4,5-F)QUINOXALINE; 2-AMINO-6-METHYLDIPYRIDO(1,2-A:3',2'-D)IMIDAZOLE; 2-AMINO-9H-PYRIDO(2,3-B)INDOLE; 3-AMINO-1-METHYL-5H-PYRIDO (4,3-B) INDOLE; 3-AMINO-1,4-DIMETHYL-5H-PYRIDO (4,3-B) INDOLE 76180-96-6 (2-AMINO-3-METHYLIMIDAZO(4,5-F)QUINOLINE) REGISTRY NUMBER: 62450-07-1 (3-AMINO-1-METHYL-5H-PYRIDO(4,3-B)INDOLE) 486-84-0 (HARMAN) 244-63-3 (NORHARMAN) 62450-06-0 (3-AMINO-1,4-DIMETHYL-5H-PYRIDO(4,3-B)INDOLE) 67730-11-4 (2-AMINO-6-METHYLDIPYRIDO(1,2-A:3',2'-D) IMIDAZOLE) 77094-11-2 (2-AMINO-3,4-DIMETHYLIMIDAZO(4,5-F)QUINOLINE)

77500-04-0 (2-AMINO-3,8-DIMETHYLIMIDAZO(4,5-F)QUINOXALINE)

61.07 61.28

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